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On the computation of the demagnetization tensor for particles of arbitrary shape

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Abstract

A new method is presented to compute the demagnetization tensor of particles of arbitrary shape. By means of a Fourier space approach it is possible to compute analytically the Fourier representation of the demagnetization tensor for a broad class of magnetic nanoparticles. Then, specifying the direction of the uniform magnetization, the demagnetizing field and the magnetostatic energy associated with the particle can be evaluated.

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The calculation of the demagnetization tensor field N_{ij} is of fundamental importance for a quantitative analysis of the energy associated with a particular magnetization state of a magnetized particle. Micromagnetic simulations rely on the numerical evaluation of N_{ij}, often with strong assumptions about the geometry of the computational cell. A complete theoretical scheme for the computation of the preferred magnetization direction as a function of particle shape in uniformly magnetized nanoparticles is still lacking.

Using a new Fourier space formalism, N_{ij} can be computed for a broad class of geometries, namely the faceted (polyhedral) particles and some selected high-symmetry shapes (solids with a rotation axis or some symmetry plane). For both classes of particles, the demagnetization tensor field can be written in analytical form in Fourier space, and a numerical or analytical inverse transform results in the tensor field in real space. For the rotational solids, the Fourier inversion is sometimes computable analytically, at least to reduce the dimensionality of the numerical iFFT.

It is worth emphasizing that the method presented here is of general validity, and does not rely on any assumptions or simplifications. This formalism may contribute to a significant improvement of the accuracy of micromagnetic simulations, as well as lead to a new fundamental understanding of the magnetic properties of nanoparticles.

The shape of a particle can be described mathematically by means of the characteristic function or shape function, a function which is equal to unity inside the particle and vanishes outside. It was shown in Ref. [1] how to evaluate the Fourier representation of the shape function $D(\mathbf{k})$ for a faceted particle. Then, in Ref. [2], this scheme was applied to the calculation of the vector potential and the electron-optical phase shift experienced by a plane electron wave traveling around and through the magnetized particle. The same approach, adapted to the analysis of magnetized nanoparticles, is employed here in order to calculate analytically the Fourier space representation of the N_{ij} tensor field, which can be written as

$$N_{ij}(\mathbf{k}) = \frac{D(\mathbf{k})}{k^2} k_i k_j. \tag{1}$$

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The magnetostatic energy can be evaluated within the Fourier space approach without involving explicitly the demagnetization tensor N_{ij}:

$$E_m = \frac{\mu_0 M_0^2}{16\pi^3} \int d^3\mathbf{k} \frac{|D(\mathbf{k})|^2}{k^2} (\mathbf{m} \cdot \mathbf{k})^2, \quad (2)$$

where $\mathbf{m}$ is the magnetization unit vector, and M_0 is the magnetization amplitude.

As an example computation, we analyze the case of a cylindrical particle of radius R, thickness $t = 2d$ and aspect ratio $\tau = t/2R$. The shape amplitude is given by [3]

$$D(\mathbf{k}) = \frac{4\pi R}{k_\perp k_z} J_1(k_\perp R)\sin(dk_z). \quad (3)$$

The demagnetization tensor is then directly obtained in Fourier space from Eq. (1). The inversion in real space of N_{ij} is cumbersome but feasible, and the complete expression will be presented elsewhere [4]. We can derive the expression for the magnetostatic energy, from Eq. (2) is

$$E_m = \frac{E_m}{\mu_0 M_0^2 V} = \frac{1}{2} m_z^2 + \frac{3m_z^2 - 1}{\tau} \times \left[\frac{1}{3\pi} - \frac{\sqrt{1+\tau^2}}{4} {}_2F_1\left(-\frac{1}{2}, \frac{3}{2}, 2, \frac{1}{1+\tau^2} \right) \right]. \quad (4)$$

In this equation, V represents the cylinder volume, m_z the vertical component of the magnetization, and ${}_2F_1$ is a hypergeometric function. The energy is shown in Fig. 1 as a function of the cylinder aspect ratio τ and the magnetization azimuthal angle θ. The energy surface shows a saddle-point at $\tau = 0.9065$ and $\theta = 35.26°$. For smaller aspect ratios, the magnetization prefers to be normal to the cylinder axis (in-plane), while for larger aspect ratios the magnetization lies along the cylinder axis.

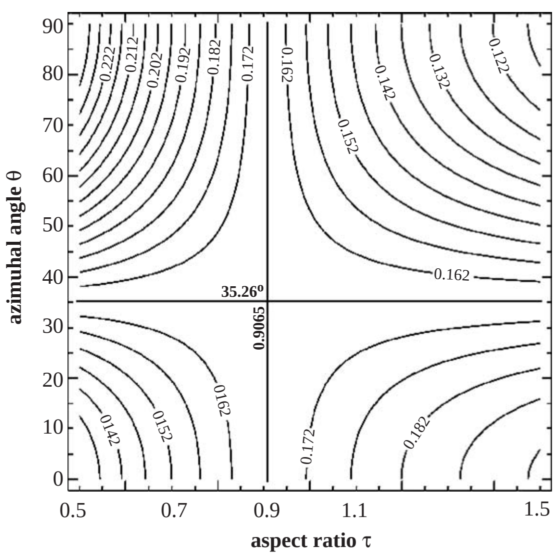

Fig. 1. Magnetostatic energy of a cylindrical particle with an aspect ratio τ and a magnetization azimuthal angle θ.

The explicit computation of the demagnetization tensor field of the uniformly magnetized cylinder, presented in Ref. [4], leads to a graphical representation of the tensor field in terms of ellipsoids, shown in Fig. 2. The eigenvectors and eigenvalues of the tensor provide the orientation and length of the major axes of the ellipsoids for points inside the cylinder. For all external points, the sum of the eigenvalues vanishes, so that the corresponding quadratic surface must be a single- or a double-sheet hyperboloid. The major axes of the hyperboloids are indicated by short rods, with length equal to the modulus of the eigenvalue. For negative eigenvalues, the rod is represented in a lighter color. This representation of the tensor field can be used to determine the magnetic field around the cylinder for an arbitrary magnetization direction [5].

In order to make progress in the research on magnetic materials, this theoretical framework must be tested against experiment and employed to measure physical quantities. Transmission electron microscopy experiment will be carried out in the near future with nanoparticles of well defined geometry or magnetic structures of interest. Electron holography and related phase retrieval techniques may enable us to access the information regarding magnetic fields around the particles or structures. Such information would be

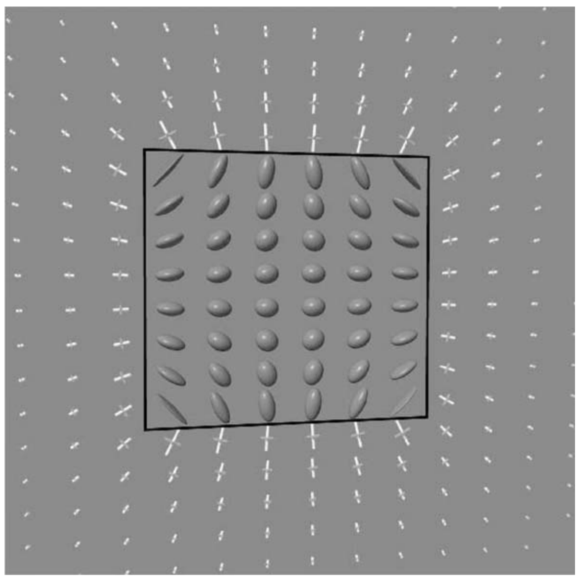

Fig. 2. Three-dimensional perspective representation of the demagnetizing tensor for a cylindrical particle with unit aspect ratio. The drawing represents a planar cut containing the cylinder axis (vertical direction).

suitable for a thorough comparison with the results of the calculations presented here.

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